## The polymeric anhydrous rubidium hydrogen oxalate

M. Hamadène, H. Kherfi, A. Guehria-Laidoudi

*Faculté de Chimie, U.S.T.H.B., BP 32 El-Alia, Bab-Ezzouar, Alger, Algerie.
e-mail:mal_hamadene@hotmailcom.*

**Keywords: crystal structure, strong hydrogen bond, polymeric dicarboxylate**

The anhydrous complex of the rubidium hydrogen oxalate has been synthesized as single crystal and characterized by X-ray diffraction, IR spectroscopy and thermogravimetric study. The structure has been determined from data collected on a Kappa CCD diffractometer and shows the compound to be isostuctural with the potassium hydrogen oxalate [1]: it crystallizes in space group $P2_1/c$ (Z=4) with the cell parameters a=4.2940(3), b= 13.6230(10), c=7.6689(5) and $\beta$=101.50(50)°, slightly different from those found by Hendricks [2]. The structure consists of layers formed by chains of one-edge-sharing rubidium polyhedra, running along the [001] direction and alternating layers of hydrogen oxalate groups, Hox, which are hydrogen bonded. The rubidium atom is sevenfold coordinated with two bridged-chelating Hox ligands and three bridged monodendate hydrogen oxalate.

As expected, the anion group is non planar and is found to be twisted about the C-C bond with an angle of about 15°. It is due to the strong hydrogen bond which is usual in acid salt alkali metal and hydrogeno-carboxylates complexes [1][3][4][5]. This hydrogen bond O-H ....O' which connects the hydrogen oxalate ions is asymmetric (O-H and H ...O' distances are respectively 0.99 and 1.547Å) and approximately linear (the O-H ...O' angle is 176°).

The IR spectrum shows the bands due to the free carboyl absorption and to oxalate salts as the bands of O-H streching modes and the thermal decomposition agrees with the XR and IR investigations.

[1] H. Einspahr, R.E. March, Acta Cryst., B28, (1972) 2194.
[2] S.B. Hendricks, Z. Kristallogr. 91 (1935) 48.
[3] R. Tellgren, J.O. Thomas, I. Olovsson, Acta Cryst., B33 (1977) 3500.
[4] R.G. Delaplane, R. Tellgren, I. Olovsson, Acta Cryst., C40 (1984) 1800.
[5] B. Benmerad, A. Guehria-Laïdoudi, F. Balegroune, H. Birkedal, G. Chapuis, Acta Cryst., C56 (2000) 789.

## Structural class distribution for *cis/trans*-PtX$_2$L$_2$, X=halogen, L=neutral ligand; the structures of two polymorphs of *cis*-PtCl$_2$(Bz$_2$S)$_2$

Christian Hansson, Åke Oskarsson

*Organic chemistry, Centre for Chemistry and chemical engineering, Lund University, PO Box 124, SE-221 00 Lund, Sweden*

**Keywords: coordination crystal chemistry, structural class, packing analysis**

The structural class concept [1] carries information about point group symmetry and may thus be used to answer the question: What point group symmetry is retained in the solid state? Such common features will be of most interest for molecules that have similar crystallochemical nature, like *cis/trans*-PtX$_2$L$_2$; X = halogen, L = neutral ligand. *trans*-PtX$_2$L$_2$ may adopt point groups $C_1$, $C_s$, $C_2$, $C_{2v}$, $C_i$ and $C_{2h}$, while *cis*-PtX$_2$L$_2$ is constrained to $C_1$, $C_s$, $C_2$ and $C_{2v}$. The most frequently observed molecular point group for complexes *trans*-PtX$_2$L$_2$ is $C_i$ (78%) followed by $C_1$ (16%) [2]. Even if *cis*-PtX$_2$L$_2$ cannot adopt to $C_i$ it often forms a centrosymmetric dimeric packing arrangement in the solid state. The dimers as observed in the Cambridge Structural Database (2005 release) [3] are classified according to the interaction across the centre of symmetry formed by two i) Pt---X, ii) Pt---L (donor atom), iii) Pt---L (hydrogen atom) and iv) Pt---L (other type) interactions. In many cases the interaction between the complexes forming dimers seems to be small, but in some cases it is of chemical significance. Two polymorphs of *cis*-PtCl$_2$(Bz$_2$S)$_2$ crystallizing in P-1 and C2/c, respectively, have been synthesized. The polymorph in C2/c is more close-packed (D$_x$=1.67 g/cm$^3$) than the one in P-1 (D$_x$=1.61 g/cm$^3$) in conflict with Kitaigorodsky ́s division of space groups into closest-packed, limiting close-packed, permissible and impossible [4], where P-1 belongs to closest-packed and C2/c permissible. However, it is in agreement with Wilson ́s idea [5], that by introducing centrosymmetric dimers in the packing description, C2/c is moved from permissible to closest-packed. Structural class frequencies for *cis*-PtX$_2$L$_2$ as observed in CSD will be reported and discussed.

[1] Belsky, V. K., Zorkaya, O. N. & Zorky, P. M. (1995). *Acta Cryst.* A51, 473-481.
[2] Hansson, C., Carlson, S., Giveen, D., Johansson, M., Yong, S. & Oskarsson, Å. (2006). *Acta Cryst B* (accepted)
[3] Allen, F. H. (2002). *ActaCryst.* B38, 380-388.
[4] Kitaigorodsky, A. I. (1973). Molecular Crystals and Molecules. Academic Press, New York & London.
[5] Wilson, A. J. C. (1993). *Acta Cryst*. A49, 210-212.